

Universal property of the information entropy in atoms, nuclei and atomic clusters

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The position- and momentum-space information entropies of the electron distributions of atomic clusters are calculated using a Woods-Saxon single particle potential. The same entropies are also calculated for nuclear distributions according to the Skyrme parametrization of the nuclear mean field. It turns out that a similar functional form $S = a + b \ln N$ for the entropy as function of the number of particles N holds approximately for atoms, nuclei and atomic clusters. It is conjectured that this is a universal property of a many-fermion system in a mean field. It is also seen that there is an analogy of our expression for S to Boltzmann's thermodynamic entropy $S = k \ln W$.

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Information-theoretical methods have played in recent years an important role in the study of quantum mechanical systems [1–9] in two cases: first in the clarification of fundamental concepts of quantum mechanics and second in the synthesis of probability densities in position and momentum spaces. In the first case an important step was the discovery of an entropic uncertainty relation (EUR) by Bialynicki-Birula and Mycielski [1] which for a three-dimensional system has the form:

$$S_r + S_k \geq 3(1 + \ln \pi), \quad (\hbar = 1) \quad (1)$$

(see also ref. [10] for the one-dimensional case). In (1) S_r is the Shannon information entropy in position-space:

$$S_r = - \int \rho(\vec{r}) \ln \rho(\vec{r}) d\vec{r} \quad (2)$$

S_k is the corresponding entropy in momentum-space:

$$S_k = - \int n(\vec{k}) \ln n(\vec{k}) d\vec{k} \quad (3)$$

and $\rho(\vec{r})$, $n(\vec{k})$ are the position- and momentum-space density distributions respectively, which are normalized to one. However, for a normalization to the number of particles N , the following EUR holds [4]:

$$S_r + S_k \geq 3N(1 + \ln \pi) - 2N \ln N = 6.434N - 2N \ln N \quad (4)$$

Inequality (1), for the information entropy sum in conjugate spaces, is a joint measure of uncertainty of a quantum mechanical distribution, since a highly localized $\rho(\vec{r})$ is associated with a diffuse $n(\vec{k})$, leading to low S_r and high S_k and vice-versa. Expression (1) is an information-theoretical uncertainty relation stronger than Heisenberg's [1]. We also note that expression (1)

does not depend on the unit of length in measuring $\rho(\vec{r})$ and $n(\vec{k})$ i.e. the sum $S_r + S_k$ is invariant to uniform scaling of coordinates.

Gadre [2] derived the following approximate expression for the information entropies of electron distributions in atoms:

$$S_r + S_k \simeq 6.65N - N \ln N \quad (5)$$

using Thomas-Fermi theory and Gadre et al [3] derived :

$$S_r + S_k \simeq 6.257N - 0.993N \ln N \quad (6)$$

with Hartee-Fock calculations. Here, N is the number of electrons.

Panos and Massen [8] found the following expression for nuclear distributions, employing the simple harmonic oscillator (HO) model of the nucleus:

$$S_r + S_k \simeq 5.287N - 1.13N \ln N \quad (7)$$

where N is the number of nucleons in nuclei. Relations of the same functional form hold for S_r and S_k separately but the important quantity is $S_r + S_k$.

There is a striking similarity of (5), (6) and (7) with the EUR (4), indicating that the functional form

$$S = aN + bN \ln N \quad (8)$$

is universal for a many-fermion system in a mean field.

However, the above relations were derived for a normalization of $\rho(\vec{r})$ and $n(\vec{k})$ to the number of particles N . In the following we find it more convenient to normalize to one. There is a simple relationship between the two cases and we can easily transform one case to the other according to the relations:

$$S_r[norm = 1] = \frac{S_r[norm = N]}{N} + \ln N$$

$$S_k[norm = 1] = \frac{S_k[norm = N]}{N} + \ln N$$

Hence, we have for normalization to one, the following expressions:

$$S_r + S_k \simeq 6.65 + \ln N \quad (atoms, Thomas - Fermi) \quad (9)$$

$$S_r + S_k \simeq 6.257 + 1.007 \ln N \quad (atoms, Hartee - Fock) \quad (10)$$

$$S_r + S_k \simeq 5.287 + 0.870 \ln N \quad (nuclei - H.O.) \quad (11)$$

In the present letter we extend our calculations for two other cases: the distribution of the valence electrons in atomic clusters using a Woods–Saxon single particle potential and the nuclear distribution in nuclei employing the Skyrme parametrization of the nuclear mean field.

In atomic (metallic) clusters the effective radial electronic potential was derived by Ekardt [11] in his spherical–jellium–background–model study of the self-consistent charge density and the self-consistent effective one-particle potential, using the local density approximations. Ekardt’s potentials for neutral sodium clusters were parametrized in ref. [12] by a Woods–Saxon potential of the form:

$$V_{WS}(r) = -\frac{V_0}{1 + \exp[\frac{r-R}{a}]} \quad (12)$$

with $V_0 = 6 \text{ eV}$, $R = r_0 N^{1/3}$, $r_0 = 2.25 \text{ Å}$ and $a = 0.74 \text{ Å}$. For a detailed study regarding the parametrization of Ekardt’s potentials see ref. [13].

We solved numerically the Schrödinger equation for atomic clusters with $Z = 8, 18, 20, 34, 40, 58, 68, 70$ valence electrons in the potential (12) and found the wave functions of the single-particle states in configuration space and by Fourier transform the corresponding ones in momentum space. Using the above wave functions, we calculated the electron density $\rho(\vec{r})$ in position space and $n(\vec{k})$ in momentum space, which were inserted into equations (2), (3) and gave us the values of the information entropies S_r and S_k . Then we fitted the form $S = a + b \ln N$ to these values and obtained the expressions:

$$S_r \simeq 4.133 + 0.934 \ln N \quad (13)$$

$$S_k \simeq 1.563 - 0.027 \ln N \quad (14)$$

$$S_r + S_k \simeq 5.695 + 0.907 \ln N \quad (15)$$

Next the nuclear densities $\rho(\vec{r})$ and $n(\vec{k})$ for several nuclei were obtained with Hartee–Fock calculations using the Skyrme parametrization of the nuclear mean field. There are various parametrizations of the Skyrme interaction, but they affect slightly the information entropies [9]. Thus we used the SKIII interaction [14]. Finally, we fitted the form $S = a + b \ln N$ to the values obtained with SKIII interaction and we found the expressions:

$$S_r \simeq 3.395 + 0.767 \ln N \quad (16)$$

$$S_k \simeq 1.929 + 0.091 \ln N \quad (17)$$

$$S_r + S_k \simeq 5.319 + 0.860 \ln N \quad (18)$$

The fit is in reasonably good agreement with its H.O. counterpart (comparison of relation (18) to (11)), though the individual entropies S_r and S_k do not match with the respective HO ones [8] that well. It seems that there is a delicate balance between the coordinate and momentum spaces, so that the interesting quantity is the sum $S = S_r + S_k$ (the net information content of the system) and not the individual entropies S_r and S_k .

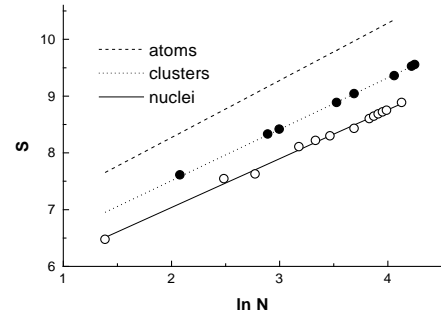


FIG. 1. Information entropy S as function of the number of particles N according to our fitted expression $S = a + b \ln N$ for atoms, clusters and nuclei. The corresponding values of our numerical calculations are denoted by solid circles (clusters) and open circles (nuclei).

In figure 1 we plot our fitted form $S = S_r + S_k = a + b \ln N$ for atoms (with Hartee–Fock, relation (10), upper curve), atomic neutral Na clusters (relation (15), middle curve) and nuclei (with Skyrme, relation (18), lower curve). These lines correspond to our fitted expressions, while the corresponding values of our numerical calculations are denoted by solid circles (clusters) and open circles (nuclei with SKIII interaction).

Concluding, in the present letter we derive an interesting characteristic of information entropies S_r and S_k for various systems i.e. atoms (Thomas–Fermi theory, Hartee–Fock), nuclei (Harmonic Oscillator model, Skyrme force) and atomic clusters (Woods–Saxon potential). For all of these systems the entropies can be represented well by a function, which incorporates $\ln N$ linearly i.e. $S = a + b \ln N$ where N is the number of electrons in atoms or nucleons in nuclei or electrons in atomic clusters. We may conjecture that this is a universal property of a many-fermion system in a mean field. As stated in ref. [3], the information entropies seem to be a hidden treasure, as yet remains mostly unexplored.

A final comment seems appropriate: There is an analogy of our expression $S = a + b \ln N$ to Boltzmann’s thermodynamic entropy $S = k \ln W$ (k is Boltzmann’s constant). This can be seen as follows: Our relation can be written in the form:

$$S = b \ln(N/N_0) \quad (19)$$

where $1/N_0 = e^{a/b}$. The above entropy is the information entropy S_{inf} , which is related to the physical entropy S_{phys} through Jaynes’ relation: $S_{phys} = k S_{inf}$. In our case, we have:

$$S_{phys} = kb \ln(N/N_0) \quad (20)$$

Here b and N_0 depend on the system under consideration (atom, cluster or nucleus), but this dependence is not strong. One can take that $b \approx 1$ (actually equals 1.007 for atoms, 0.907 for clusters and 0.860 for nuclei) and $1/N_0 \approx 500$ (because $1/N_0 = 500$ for atoms, 485 for nuclei and

533 for clusters). Thus we obtain the following rough estimate for the entropy of a many-fermion system:

$$S_{phys} \approx k \ln(500N) \quad (21)$$

The number $500N$ corresponds to the number of equiprobable microstates W of Boltzmann's relation.

Hence, starting from Shannon's information entropies of quantum-mechanical distributions, we arrived at relation (21), which can be considered as a quantum-mechanical analogue to Boltzmann's entropy $S = k \ln W$.

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